National Center for Computational Sciences Snapshot The Week of July 2, 2007

Simulation Helps Unlock the Ocean's Secrets

Project looks into the fate of trapped heat and greenhouse gases

Climate scientists are using the NCCS's Cray XT4 Jaguar supercomputer to illuminate the ocean's role in regulating climate.

The job is enormous. The earth is enveloped by 319 million cubic miles of ocean, which covers nearly three-quarters of the planet to an average depth of more than 12,000 feet. Ocean currents help determine which regions will be frigid and which will be temperate, which will be jungle and which will be desert. The ocean holds vast amounts of heat, as well as carbon dioxide and other greenhouse gases, and it plays a pivotal role in the earth's climate on timescales from years to millennia.

Nevertheless, our understanding of how the ocean plays its part is limited at best. A team led by Synte Peacock of the University of Chicago is using Jaguar's massive power to run the most fine-grained, global-scale simulations ever of how the oceans work. In doing so, the team will not only provide new knowledge of the currents and processes at work in the oceans, but also details about the possible long-term fate of gases—especially the greenhouse gas carbon dioxide—and chemicals released into the ocean.

"We don't yet really understand the role of the ocean in regulating climate," Peacock explained. "For example, only about half of the carbon dioxide that has been emitted over the last 100 years or so currently resides in the atmosphere. The rest is in the ocean and the terrestrial biosphere. But the absolute amount stored in the ocean, and how it is distributed, is still being debated."

The team is performing the first-ever 100-year simulation of the ocean at a fine enough scale to include the relatively small, circular currents known as eddies. Eddies play a key role in the dynamics of the ocean, but until recently researchers lacked the computing power to directly simulate eddies on a global scale.

The team's ocean model will eventually be incorporated into a fully eddy-resolving version of the Community Climate System Model, a global climate model being developed primarily by researchers at the National Center for Atmospheric Research. According to Peacock, this will be the first time that a coupled climate model will include an ocean able to resolve eddies.

The information it provides will be extremely valuable for climate scientists and policy makers alike because a reliable ocean model is critical to a reliable climate model. By helping us understand how the ocean handles the massive amounts of heat and greenhouse gases it contains, Peacock's team will aid us in becoming more knowledgeable and responsible guardians of the planet.

Striking the Perfect Balance

Solving the riddles of fusion power production

Researchers are using the NCCS's leadership computing systems to model heat and particle loss in a fusion reactor, paving the way for a clean, abundant form of energy.

A team led by Jeff Candy of General Atomics is using the NCCS systems to focus on the ionized gas—known as plasma—that serves as a reactor's fuel. The plasma generates energy when hydrogen atoms within it collide, creating high-energy alpha particles and neutrons. Eventually, the reactor reaches a temperature ten times that of the sun.

According to Candy, the plasma is turbulent, and this turbulence is extremely difficult to simulate. It causes the reactor to lack "perfect containment"— as the alpha particles heat the plasma, turbulence carries some of the heat away and eventually throws out the particles—but it is also necessary.

The key, says Candy, is to know the rate at which the plasma is leaking heat and particles. With that knowledge, researchers can find "optimum turbulence," the perfect balance of heat and alpha-particle production and loss.

Candy's team is pursuing this perfect balance with his revolutionary GYRO code, which, among other things, calculates electromagnetic fluctuations in fusion plasmas. The code simulates a tokamak, which is a doughnut-shaped fusion reactor such as the international ITER project and leading research reactors.

The team is also developing a new type of code designed to advance the quest for optimum turbulence. The new code will predict the operating temperatures and densities in a reactor by designing a feedback loop that uses multiple GYRO calculations.

"Gyrokinetic simulations are a bit like a black box," Candy explains. "You tell it what the densities and temperatures are, and it will tell you how violent the turbulence is. By introducing feedback schemes, you find the unique temperatures and densities for which heat loss balances heat production. That's never been done before using gyrokinetic simulations."

Fortunately, he said, the project is able to take full advantage of the growing computing power offered at the NCCS. While the simulations will take up to 100 times the processing power of previous work, the GYRO code is able to take advantage of the thousands of processors available on the center's state-of-the-art supercomputers.

Students Taste the Joys of Supercomputing

Crash course gives them the tools to get started

Supercomputing's next generation gathered at ORNL's Joint Institute for Computational Sciences June 19 to get a taste of leadership computing on the NCCS's IBM Cheetah system.

About 40 graduate students and undergraduates—pursuing careers in math, chemistry, physics, biology, and computer science—attended "A Crash Course in Supercomputing" taught by Rebecca Hartman-Baker of ORNL's Computer Science and Mathematics Division. In it, they were able to sample computing at a level unavailable in the typical college environment.

Hartman-Baker introduced students to the UNIX operating system and tools for writing the highly parallel programs required by modern high-performance computers. The course also included a tour of the NCCS and the Everest visualization facility. Hartman-Baker, who noted that the tours helped make the material covered in the course seem more concrete, credited Don Frederick of the NCCS's User Assistance and Outreach Group with helping to arrange both the tours and the students' access to Cheetah.

Fisk Junior Working to Make Jaguar Purr

Computer science major spending summer at NCCS through RAMS program

Fisk University junior Joylika Adams is working to make the NCCS's premier Jaguar supercomputer the most effective tool possible.

Adams, a major in computer science, is working with Mark Fahey of the NCCS's Scientific Computing Group through the Research Alliance in Math and Science (RAMS). Her work promises to help Jaguar users by identifying the most effective methods for performing input and output on the system.

The RAMS program works with universities to provide opportunities for underrepresented minorities and promote diversity within computational science. Fisk has been a long-time participant in the program, according to ORNL principal investigator Debbie McCoy, and university faculty regularly have summer appointments at ORNL.

While Adams's summer project focuses on Jaguar's Cray XT3/XT4 architecture, Fahey noted that some of the information she is developing might well be useful in any high-speed file system.